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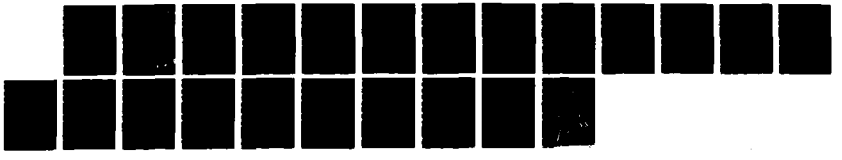

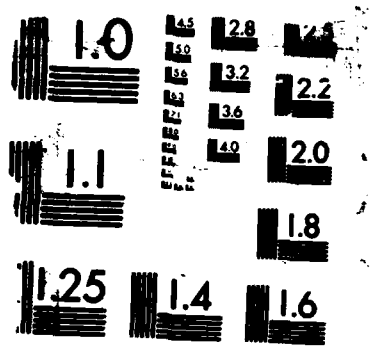

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David P. Pope, Harry A. Lipsitt and Alexander Cruickshank

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The 1987 Gordon Conference in Physical Metallurgy concerned the subject of "Intermetallic Compounds". The Conference was held at Tilton School, Tilton, N.H., 20-24 July 1987. The Conference consisted of papers presented by authors outstanding in the field and of extensive discussion. The Conference was attended by 130 scientists and engineers from the USA and from seven other countries.

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FINAL REPORT

AFOSR GRANT (AFOSR-87-0195) FOR THE SUPPORT OF THE
1987 GORDON CONFERENCE ON PHYSICAL METALLURGY

"INTERMETALLIC COMPOUNDS"

Submitted to

Air Force Office of Scientific Research
Division of Research Grants, Building 410
Bolling AFB, Washington, D.C. 20332

Attention: Dr. Alan H. Rosenstein

Submitted by

Dr. David P. Pope (Co-Chairman and P.I.)
Associate Dean, Undergraduate Education
School of Engineering and Applied Science
University of Pennsylvania
Philadelphia, PA 19104-6391

Dr. Harry A. Lipsitt
Professor, Materials Science and Engineering
Department of Mechanical Systems Engineering
Wright State University
Dayton, Ohio 45435-0001

and

Dr. Alexander M. Cruickshank (Director)
Gordon Research Conferences
Pastore Chemical Laboratory
University of Rhode Island
Kingston, RI 02881

October, 1987

INTRODUCTION

The 1987 Gordon Research Conference on Physical Metallurgy was held 20-24 July 1987 at the Tilton School, Tilton, New Hampshire. The conference topic was "Intermetallic Compounds". U.S. Government Grants were made to the Gordon Research Conference to partially offset the travel and registration costs of many of the speakers and discussion leaders, a few attendees, and the co-chairmen. The grants totalled $18,000.00. Of this total, $6000.00 each was provided by AFOSR and ONR (AFOSR-87-0195), and DOE/ECUT (DEFG05-87CE90006). In addition, $3000.00 was received from industry for this same purpose. Of this total, $2000.00 was received from the Aluminum Company of America and $1000.00 was received from the General Electric Corporation. In this report we give a brief description of the Conference and describe some of the highlights of the meeting.

CONFERENCE DESCRIPTION

The primary purpose of the Conference was to bring together three rather disparate groups: scientists and engineers concerned with the mechanical properties of intermetallic compounds, theoreticians interested in the problems of alloy stability and the calculation and prediction of the effects of chemical composition on alloy stability, and engineers interested in developing and producing new alloys based on intermetallic compounds for elevated temperature service. It is important that the → to page VI effectiveness and progress of this last group depends critically on the results of the efforts of the first two groups.

The Conference was organized to allow each group the opportunity to present the status of current work in their respective areas and to discuss their current needs. For example, on one day the theoreticians described their approach and the sort of results that were developed by that approach. On the next day, the alloy designers described how useful

alloys are <u>really</u> developed and indicated the type of information they believed the theoreticians should be producing so as to provide the maximum theoretical guidance to the alloy developers. The lengthy, animated discussions that followed indicated that much progress has been made to attune the theoreticians to the needs of the engineers and that considerable very useful information was emerging from the several existing collaborative areas. However, it continued to be clear that the most demanding needs of the engineers, i.e., predictive theories for the development of multiphase alloys, could not yet be met. It was equally clear that considerable dialogue had occured between these groups and that the theoreticians were moving rapidly toward the goal of total group integration concerning these mutually challenging problems.

Following the tradition of previous Gordon Conferences, a relatively small number of speakers were invited to make presentations to the Conference. The primary purpose of these talks was to describe recent progress and to set the stage for thought and discussion. A copy of the program of speakers and discussion leaders is appended to this report.

A poster session was also held during the Conference so that some of the participants could present their research results. This was a well attended session that provided the basis for broad exposure of very new results and stimulated a great deal of excitement that continued past midnight. A list of the poster presentations is also appended to this report.

The Conference attracted participants from a wide variety of institutions and backgrounds. The list of attendees appended to this report shows that a total of 130 scientists and engineers participated in the Conference. Of these, only 32 were on the program as speakers and discussion leaders! The attendees included 109 from the United States and

21 from foreign countries. Of these, 65 were from universities, 35 from government laboratories or offices, and 30 from industry. Finally, it is worth noting that the number of applicants for this Conference exceeded the number of places available.

PROGRAM HIGHLIGHTS

The major opportunity at a Gordon Conference is the opportunity to interact on an informal level with a large number of scientists interested and knowledgeable in a given subject. The facilities at the Tilton School catered to this aspect in a number of ways. The main lounge, the game/clubroom, pool area, and the grounds were outstanding sites for informal discussion. These facilities were in use throughout the day and night for many, many small group discussions which led to the development of new research ideas, to several future small group research interactions, and to the development of two research plans to be submitted for Government support. Thus, the informal aspect of this Gordon Conference was a rousing success.

In the more formal program, Lipsitt set the tone for the first two sessions with a critical review of the nature of the changes in mechanical properties accompanying ordering and by pointing out those areas where our understanding was weakest. Vitek described the complex structure of the dislocation core in intermetallics as well as the mechanisms by which core geometry affects deformation behavior. Yoo, building on the understanding generated by Vitek and others, introduced a totally new "mechanics" concept of the strengthening caused by dislocations in intermetallic compounds. This exciting concept provoked much thought and discussion. Later, Stoloff described recent results on fatigue, while Yamaguchi reviewed his recent experiments aimed at introducing ductility into one class of intermetallic alloys.

On the second day, Dimiduk showed that considerable understanding of ductile-brittle behavior could be gained by considering the presence or absence of a second phase in the grain boundaries, in antiphase domain boundaries, and perhaps even dispersed in the structure. This was a new concept for intermetallics with immediate effects on potential alloy development! The papers by Taub and by Izumi described a number of studies related to the atomic structure of grain boundaries and its effect on ductility. Taub's studies were very carefully done and the results cast doubt on a number of previous elementary explanations of the role of grain boundaries on deformation in intermetallics. The results presented by Williams and by Schulson were exciting because they showed how important microstructural manipulation could be as an effective way to alter mechanical behavior in these materials.

The third day belonged to the theoreticians. It was their opportunity to present the advantages and disadvantages of their individual approaches to intermetallic structures and properties. In this session, Freeman presented a particularly valuable paper showing how his ab initio ground state calculations could predict structural stability and alloying effects in intermetallics. Later, two very different (and heretical) approaches were presented by Vvedensky and by Pettifor. These two papers were the subject of the most intense discussion of the Conference. The theorectical presentations at this Conference created considerable excitement because they were given following the presentation of considerable background and because many in the audience were aware that theoretical guidance is sorely needed in the development of intermetallics for use as structural materials.

Next, several prominent engineers outlined their individual approaches to the determination of how intermetallics may best be selected for study

and modified for service. Finally, three groups that had actual experience developing intermetallic alloys described their approaches and results. The final paper of the Conference, presented by Blackburn, was the first public report on the approaches used for development of alloys based on the titanium aluminides. Since these alloys are soon to enter turbine engine service in military engines and are also prime candidates for the structure of the National Aerospace Plane, this was another paper that generated considerable interest. By actual count, 90 delegates were present to hear this final paper of the Conference.

1987 GORDON CONFERENCE ON PHYSICAL METALLURGY

July 20-24, 1987, Tilton School, Tilton, NH

TOPIC: INTERMETALLIC COMPOUNDS

H. Lipsitt and D. Pope, Co-chairs

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Monday, July 20 **Morning session**	Session Chair: G. Sauthoff Max-Planck Institüt fur Eisenforschung
8:45-9:00	WELCOME
9:00-9:40	**OVERVIEW OF STRENGTH AND DUCTILITY OF INTERMETALLIC COMPOUNDS**, H. Lipsitt Wright State University
9:40-10:00	DISCUSSION
10:00-10:30	BREAK and PHOTO SESSION
10:30-11:10	**DISLOCATION CORE STRUCTURE AND SLIP SYSTEMS IN INTERMETALLIC COMPOUNDS**, V. Vitek University of Pennsylvania
11:10-11:30	DISCUSSION
11:30-12:10	**STRENGTHENING MECHANISMS IN INTERMETALLIC COMPOUNDS**, M. Yoo Oak Ridge National Laboratory
12:10-12:30	DISCUSSION
Monday, July 20 **Evening session**	Session Chair: T. Suzuki Tokyo Institute of Technology (ANNOUNCEMENT OF NOMINATING COMMITTEE FOR CHAIR OF 1989 CONFERENCE)
7:30-8:10	**CREEP AND FATIGUE OF INTERMETALLIC COMPOUNDS**, N. S. Stoloff Rensselaer Polytechnic Institute
8:10-8:30	DISCUSSION
8:30-9:10	**DEFORMATION OF NON-CUBIC INTERMETALLIC COMPOUNDS** M. Yamaguchi Kyoto University
9:10-9:30	DISCUSSION

Tuesday, July 21 **Morning session**	**Session Chair:** **L. A. Johnson** **General Electric Corporation**
9:00-9:40	**OVERVIEW OF BRITTLE-DUCTILE TRANSITION MECHANISMS** D. Dimiduk Wright Patterson Air Force Base
9:40-10:00	DISCUSSION
10:00-10:15	BREAK
10:15-10:55	**MECHANISMS OF DUCTILITY IMPROVEMENT IN $L1_2$ COMPOUNDS** O. Izumi Tohoku University
10:55-11:15	DISCUSSION
11:15-11:55	**EFFECTS OF COMPOSITION ON THE TENDENCY FOR INTERGRANULAT FRACTURE IN $L1_2$ COMPOUNDS** A. I. Taub and C. L. Bryant General Electric Corporation
11:55-12:15	DISCUSSION

Tuesday, July 21 **Evening session**	**Session Chair:** **P. Veyssiere** **Universite de Poitiers**
	(NOMINATING COMMITTEE PRESENTS NOMINEES AND NOMINATIONS FROM FLOOR)
7:30-8:05	**MICROSTRUCTURAL EFFECTS ON THE DUCTILITY OF INTERMETALLIC COMPOUNDS** J. C. Williams Carnegie Mellon University
8:05-8:20	DISCUSSION
8:20-8:55	**GRAIN BOUNDARY ACCOMODATION OF SLIP** E. M. Schulson Dartmouth College
8:55-9:10	DISCUSSION
9:10-9:45	**GRAIN BOUNDARY MODELLING** → page XIII D. Srolovitz and S.-P. Chen Los Alamos National Laboratory
9:45-10:00	DISCUSSION

Wednesday, July 22 **Morning session**	**Session Chair:** **A. Gonis** **Northwestern University**
8:45-9:25	**LIMITATIONS AND APPROXIMATIONS OF ELECTRONIC STRUCTURE CALCULATIONS,** **A. Shere** **SRI International**
9:25-9:45	**DISCUSSION**
9:45-10:00	**BREAK**
10:00-10:40	**AB-INITIO GROUND STATE CALCULATIONS** **A. J. Freeman** **Northwestern University**
10:40-11:00	**DISCUSSION**
11:00-11:40	**THE THERMODYNAMICS OF EXTENDED DEFECTS IN INTERMETALLIC COMPOUNDS,** **J. M. Sanchez** **Columbia University**
11:40-12:00	**DISCUSSION**
12:00-12:30	**ELECTION OF CHAIR OF 1989 GORDON CONFERENCE**

Wednesday, July 22 **Afternoon session**	
4:30-6:00	**POSTER SESSION**

Wednesday, July 22 **Evening session**	**Session Chair:** **A. Sutton** **University of Oxford**
7:30-8:10	**QUANTUM MECHANICS AND FRACTURE** **D. D. Vvedensky** **Imperial College**
8:10-8:30	**DISCUSSION**
8:30-9:10	**QUANTUM MECHANICS AND ALLOY DESIGN** **D. Pettifor** **Imperial College**
9:10-9:30	**DISCUSSION**

Thursday, July 23 **Morning session**	**Session Chair:** **J. Tien** **Columbia University**
9:00-9:40	**ALLOY DESIGN: WHAT EXPERIMENTALISTS NEED FROM THEORETICIANS** **S. K. Das** **Allied Chemical Corporation**
9:40-10:00	**DISCUSSION**
10:00-10:15	**BREAK**
10:15-10:55	**SELECTION AND EVALUATION OF INTERMETALLIC ALLOYS** **D. M. Shah** **Pratt and Whitney Aircraft**
10:55-11:15	**DISCUSSION**
11:15-11:55	**THE SEARCH FOR HIGH STRENGTH AT HIGH TEMPERATURES** **R. L. Fleischer** **General Electric Corporation**
11:55-12:15	**DISCUSSION**

Thursday, July 23 **Evening session**	**Session Chair:** **D. P. Pope** **University of Pennsylvania**
8:30-9:30	**CORROSION AND ART** **J. E. Harris** **Berkeley Nuclear Laboratories**
9:30-10:00	**DISCUSSION**

Friday, July 24 **Morning session**	Session Chair: C. C. Koch North Carolina State University
8:45-9:25	**DUCTILE Ni-ALUMINIDE ALLOYS** C. T. Liu Oak Ridge National Laboratory
9:25-9:45	DISCUSSION
9:45-10:00	BREAK
10:00-10:40	**B2-BASE MATERIALS AND COMPOSITES** K. Vedula Case Western Reserve University
10:40-11:00	DISCUSSION
11:00-11:40	**NiAl AND TiAl-BASE ALLOYS** M. J. Blackburn Pratt and Whitney Aircraft
11:40-12:00	DISCUSSION

POSTER SESSION CONTRIBUTIONS

1. "Physical Metallurgy and Creep Properties of a Beta-NiAl + 4.5 a/o Ta Alloy", V.M. Pathare, G.M. Michal, and K.M. Vedula, Case-Western Reserve University, Cleveland.

2. Rapid Solidification of TiAl Intermetallic Compounds", J.M. Graves and J.H. Perepezko, University of Wisconsin, Madison.

3. Mechanical Properties and MIcrostructure of a Ni-Base Alloy Single Crystal", M. Mills, N. Baluc, J Bonneville, and J. Stolber, Ecole Polytechnic, Lausanne.

4. "Sigma Distribution and Relative Energy Determinations of Grain Boundaries in Ductile and Brittle Ni_3Al", Diana Farkas, M.O. Lewis, and R. Venkataraman, Virginia Polytechnic Institute, Blacksburg.

5. "Influence of Grain Boundaries on the Crack Development in Thin Foils of Ni_3Al", R. Maurer, Max Planck Inst. fur Metallforschung, Stuttgart.

6. "Strengthening of Ni_3Al by Ternary Additions", F. Heredia and D. Pope, University of Pennsylvania, Philadelphia.

7. "Dislocation Structure in Gamma Prime Strengthened Superalloy", Y.Q. Sun and P.M. Hazzledine, Oxford University, England.

8. "Plastic Deformation and Ductility Improvement of Al_3X Type Compounds of Al with the DO_{22} Structure", Y. Umakoshi, M. Yamaguchi, and T. Yamane, Tokyo.

9. "Oscillatory Relaxations in (111) Planar Defects in Ni_3Al", D. Farkas, E.J. Savino, and F. Chidamabaram, Virginia Polytechnic Inst., Blacksburg.

GORDON RESEARCH CONFERENCES

PHYSICAL METALLURGY

Tilton School, Tilton NH
July 20-24, 1987

K = Knowles
P = Pfeiffer
Bar = Barrows
Beau = Beaumont
M = Mansion

REGISTRATION LIST

Allen, Samuel 217 EK
MIT, Room 13-5056
Cambridge, MA 02139

Angers, Lynette 337 WK
Alcoa Technical Center
Alloy Technology Division
Alcoa Ctr., PA 15069

Antolovich, Stephen 228 WK
Georgia Tech., School of Materials Eng.
Fracture and Fatigue Res. Lab.
Atlanta, GA 30332-0245

Arunachalan, V.S. 129 WK
Scientific Advisor to the Minister
Ministry of Defence
South Block, P.O. New Delhi
India 11011

Banerjee, Dipankar 327 EK
Defence Metallurgical Research Lab
Structural Metallurgy Group
Hyderabad, India 500258

Birnbaum, Howard 8 P
University of Illinois
Materials Res. Lab
104 S. Goodwin Ave.
Urbana, IL 61801

Boettinger, William 332 EK
National Bureau of Standards
Metallurgy Division
Materials A153
Gaithersburg, MD 20899

Bonneville, Joel 126 WK
Ecole Polytechnique Federale Lausanne
Inst. de Genie Atomique
1015 Lausanne, Switzerland

Brenner, Sidney 31 P
University of Pittsburgh
Dept. of Materials Science & Engineering
848 Benedum Hall
Pittsburgh, PA 15261

Broderick, Thomas 301 EK
AFWAL/MLLS
Wpafb, Ohio 45433

Bryant, Daniel 325 EK
Martin Marietta Labs
1450 S. Rolling Road
Baltimore, MD 21227

Chang, Chen-Chung 247 WK
Univ. of Pennsylvania
3231 Walnut St.
Dept. MSE, Room 234
Philadelphia, PA 19104

Chesnutt, James 302 EK
General Electric
Neumann Way, M89
Cincinnati, OH 45215-6301

Chen, Shao-Ping
Los Alamos National Lab
T-11, MSB262
Los Alamos, NM 87545

Clapp, Philip 101 EK
University of Connecticut
Dept. of Metallurgy, U-136
97 N. Eagleville Road
Storrs, CT 06268

Darby, Joseph Jr. 25 P
US Dept. of Energy
Division of Materails Sciences
ER-13, G-236, GTN
Washington, DC 20545

Darolia, Ram 303 EK
General Electric Co.
1 Neumann Way, M-89
Cincinnati, OH 45215

Das, Santosh 321 E1
Allied-Signal Inc.
Metals & Ceramics Lab.
P.O. Box 1021 R
Morristown, NJ 07960

Dimiduk, Dennis 304 EK
AFWAL Materials Lab
AFWAL/MLLM
Wright-Patterson, OH 45433-6533

Don, Jarlen 322 EK
Southern Illinois University
Dept.of Mechanical Eng.
Carbondale, IL 62901

Dulmaine, Bradford 218 EK
Carpenter Technology Corp.
Research and Development
P.O. Box 14662
Reading, PA 19612-4662

Eberhardt, James 102 EK
U.S. Dept. of Energy
Energy Conversion Tech. Prog.
1000 Independence Ave., S.W. CE-12
Washington, DC 20585

Eberhart, Mark 317 EK
Los Alamos National Lab.
MS-6730, Lanl-MIT
Los Alamos, NM 87545

Farkas, Diana 336 WK
VPI & SU, Dept. of Material Engr.
202 Holden Hall
Blacksburg, VA 24061

Field, Robert 303 EK
General Electric Co.
Aircraft Engine Business Group
Mail Drop M87, 1 Newmann Way
Cincinnati, OH 45215-6301

Fleischer, Robert 128 WK
General Electric
R & D Center
Schenectady, NY 12301

Fraser, Hamish 231 WK
University of Illinois-Urbana
Dept. of Metallurgy & Mining Engr.
1304 W. Green St.
Urbana, IL 61801

Freeman, Arthur 12 P
Northwestern University
Dept. of Physics & Astronomy
2145 No. Sheridan Road
Evanston, IL 60201

Gibala, Ronald 21 P
University of Michigan
Dept. of Materials Scei & Engr.
2300 Hayward Street
Ann Arbor, MI 48109

Gibeling, Jeffery 221 EK
Dept. of Mechanical Engineering
University of California
Davis, CA 95616

Gunis, Antonios 206 EK
Chemistry & Materials Science
Lawrence Livermore National Lab.
Livermore, CA 94550

Graves, Jeffrey 326 EK
University of Wisconsin-Madison
Dept. of Met & Min. Engineering
1509 University Ave.
Madision, WI 53706

Hack, John 104 EK
Los Alamos National Lab.
MS-K765, Center for Materials Science
Los Alamos, NM 87545

Harris, John 105 EK
Berkeley Nuclear Labs
CEGB
Berkeley, England GL13 9PB

Hartig, Christian 106 EK
University of Hamburg-Harburg
Harburger Schlostrasse 20
D-2100 Hamburg 90, West Germany

Hartley, Craig 5 P
Natinal Science Foundation
DMR/MRC/MET Room 410
1800 G. Street
Washington, DC 20550

Hay, Jeffrey 324 EK
Los Alamos National Lab
T-12, MS J569
Los Alamos, NM 87545

Heckel, Richard 26 P
U.S. Dept. of Energy
ER-131, Div. of Materials Sciences
Washington, DC 20545

Hemker, Kevin 320 EK
Stanford University
Dept. of Mat. Sciences, Bldg. 550
Stanford, CA 94305

Heredia, Fernando 138 WK
University of Pennsylvania
309 S. 40th St.
Philadelphia, PA 19104

Hook, Rollin 22 P
ARMCO, Inc.
Research Center
703 Curtis St.
Middletown, OH 45043

Horton, Joe 107 EK
Oak Ridge National Lab.
Bldg. 5500-A113
Metals & Ceramics Div.
Oak Ridge, TN 37831-6376

Howell, James 19 P
E.I. Dupont de Nemours & Co.
Savannah River Lab.
Aiken, SC 29808

Izumi, Osamu 127 WK
Tohuku University
Kin-Ken
Katahira 2-1-1
Sendai, Japan 980

Jacobson, Loren 204 EK
Los Alamos National Lab.
Mail Stop G770
Los Alamos, NM 87545

Johnson, Donald W. 320 EK
ARMCO Inc.
Research and Technology
703 Curtis TS
Middletown, OH 45043

Johnson, Lyman 108 EK
General Electric Corp., R&D
P.O. Box 8
Schenectady, NY 12301

Kampe, Stephen 325 [illegible]
Martin Marietta Labs
1450 South Rolling Road
Baltimore, MD 21227

Khantha, M. 335 WK
Kirchner, Helmut 137 WK
University Wien, Inst. fur Festkorperphysik
Boltzmanngasse 5
Vienna, Austria A 7090

Koch, Carl 234 WK
North Carolina State University
P.O. Box 7907
Materials Science & Engineering Dept.
Raleigh, NC 27695

Korner, Alfred 229 WK
University of Vienna
Inst. fur Festkorper Physik
Boltzmann Gasse 5
Vienna, Austria A-1090

Koss, Donald off campus
Pennsylvania State University
Dept. of Materials Science Engr.
University Park, PA 16802

Li, Che-Yu 109 EK
Cornell University
Bard Hall, Dept. of Materials Sci & Engr.
Ithaca, NY 14850

Lin, Hui 247 WK
University of Pennsylvania
3231 Walnut St., MSE, LRSM, Room 234
Philadelphia, PA 19104

Lin, Yee-Chung 246 WK
University of Tennessee
Materials Science & Engr.
Dougherty Engineering Building
Knoxville, TN 37996-2200

Lipsitt, Harry 1 M
Wright State University
Dept. of Mechanical Systems Engr.
Dayton, OH 45435

Liu, C. T. 234 WK
Oak Ridge Nat. Lab
P.O. Box X
Oak Ridge, TN 37831-6117

Livingston, James 110 EK
General Electric Co.
Corp. Res. & Dev., Bldg, K-1, Room 1C41
Schenectady, NY 12301

London, Blair 219 EK
McDonnell Douglas Res. Labs.
Dept. 224, Bldg. 110
P.O. Box 516
St. Louis, MO 63166

MacKenize, Ross 111 EK
Cornell University
Materials Science & Engr.
Bard Hall
Iathca, NY 14853

Margolin, Harold off campus
Polytechnic University
333 Jay St.
Metallurgy & Materials Science
Brooklyn, NY 11201

Martin, Patrick 204 EK
Los Alamos National Lab
M.S. G730
Los Alamos, NM 87545

Maurer, R. off campus
Max-Planck Inst. fur Metallforschung
Inst. F. Werkstoffwissenschaften
Seestrabe 92, 7000 Stuttgart 1
Fed. Rep. Germany

McEvily, A. J. 113 EK
University of Connecticut
Metallurgy Dept., U-136
Storrs, CT 06268

McMahon, C. J. 13 P
University of Pennsylvania
Dept. of MSE, 3231 Walnut St.
Philadelphia, PA 19104

Mendiratta, Madan 115 EK
Universal Energy Systems, Inc.
4401 Dayton-Xenia Rd.
Dayton, OH

Mills, Michael 126 WK
Ecole Polytechnic Federale
Institut de Genie Atomique
1015 Ecublens
Switzerland

Miracle, Daniel 80
Airforce Materials Lab
AFWAL/MLLM
Wpafb, Ohio 54533

Moxson, Vladimir 232 WK
Texas Instruments Incorporated
5093 Stausbury Drive
Solon, Ohio 44139

Mukherjee, A. K. 7 M
University of California
Dept. of Mechanical Engr.
College of Engineering
Davis, CA 95616

Nathal, Michael 233 WK
NASA Lewis Research Ctr.
21000 Brookpark Rd., MS 49-1
Cleveland, OH 44135

Noebe, Ronald 233 WK
NASA Lewis Res. Ctr.
2100 Brookpark Rd.
M.S. 49-3
Cleveland, OH 44135

Oliver, Ben 8 B
University of Tennessee
Dept. of Materials Sce. & Engr.
Room 477, Dougherty Engr. Bldg.
Knoxville, TN 37996-2200

Oliver, Warren 3 Beau
P.O. Box X
Oak Ridge National Laboratory
Oak Ridge, TN 37932

Pank, Deborah 336 WK
Penn State University
MS 49-1, NASA Lewis Research Ctr.
Cleveland, OH 44135

Pathare, Viren 219 EK
Case Western Reserve University
Materials Science & Engineering
10900 Euclid Avenue
Cleveland, OH 44106

Perepezko, John 332 EK
University of Wisconsin-Madison
Dept. of Met. & Min Engineering
1509 University Ave.
Madison, WI 53706

Pettifor, D. G. 230 WK
Imperial College
Dept. of Mathematics
London, England SW7 2AZ

Polk, Donald — 4 Beau
ONR-Materails Division
800 N. Quincy St., Code 1131
Arlington, VA 22217

Pollock, Tresa — 338 WK
MIT, Room 1-007, 77 Mass. Ave.
Cambridge, MA 02139

Pope, David — 2 Mansion
University of Pennsylvania
220 S. 33rd St.
Philadelphia, PA 19104-6391

Porter, Wallace — 232 WK
Oak Ridge National Lab
Bldg. 4500-S, MS 140
P.O. Box X
Oak Ridge, TN 37831-6140

Raman, R. V. — 7 Beau.
GTE Lab Inc.
40 Sylan Rd., Dep. 312
Waltham, MA 02554

Rawers, James — 9 P
Bureau of Mines
P.O. Box 70, Materials Science
Albany, OR 97321

Reichman, Steven — 6 Beau.
Wyman-Gordan Company
244 Worcester St.
Research & Development
No Grafton, MA 01536

Rosenstein, Alan — 5 Beau.
Air Force Office of Scientific Res.
AFOSR/NE, Bldg. 410
Bolling AFB, DC 20332

Ruckle, Duane — off campus
Garrett Turbine Engine Company
111 South 34th St., P.O. Box 5217
Materials Engr., MS 503-4AC
Phoenix, AZ 85010

Sargent, Gordon — off campus
University of Daton
School of Engineering
300 College Park Avenue
Dayton, OH 45469

Sauthoff, G. — 18 Beau.
Max-Planck Institut fur Einsenforschung
Postfach 140-260
D-4000 Dusseldorf, Fed. Rep. Germany

Schulson, Erland — 205 EK
Dartmouth College
Hanover, NH 03755

Seastrom, Charles — 9 Beau.
Dupont Company
Chambers Works
Deepwater, NJ 08023

Shah, Dilip — 10 Beau
Pratt & Whitney
M/S 114-45
400 Main Street
East Hartford, CT 06108

Sher, Arden — 319 EK
SRI International
333 Ravenswood Ave.
Bldg. 410-42
Menlo Park, CA 94303

Skewes, Steven — 231 WK
Avco Lycoming Textron
550 S. Main St.
Dept LSM-1
Stratford, CT 06497-2452

Spaephen, Frans — 203 EK
Harvard University
29 Oxford St.
Cambridge, MA 02138

Srolovitz, David — 11 Beau
Los Alamos National Lab
MS-B262/T-11
Los Alamos, NM 27545

Stoloff, Norman — off campus
Rensselaer Polytechnic Inst.
Materials Engr. Dept.
Troy, NY 12180-3590

Sundararajan, G. — 327 EK
Defense Metallurgical Res. Lab.
Mechanical Properties Group
Hyderabad, INDIA 500258

Sanchez, J.M. 19Beau
Columbia University
School of Mines
918 Mudd
New York, NY 90027

Sun, Yongqian 220 WK
University of Oxford
Dept. of Metallurgy
Parks Road
Oxford, UNITED KINGDOM OX1 3PH

Sutton, Adrian 230 WK
Oxford University
Dept. of Metallurgy
Parks Road
Oxford, UNITED KINGDOM OX1 3PH

Suzuki, Tomoo 240 WK
Tokyo Inst. of Technology
Res. Lab of Precision Machinery
4259 Nagatsuta, Midori-Ku
Yokohama, JAPAN 227

Takasugi, Takayuki 127 WK
Tohoku University
Inst. for Materials Science
2-1-1 Katahira
Sendai, JAPAN 980

Takeyama, Masao 318 EK
Oak Ridge National Lab
Martin Marietta Energy Systems, Inc.
Metals and Ceramics Division
P.O. Box X
Oak Ridge, TN 37831-6117

Taub, Alan 128 WK
General Electric
Corp. Res. & Dev. Center
P.O. Box 8, K-1/265MB
Schenectady, NY 12301

Thoma, Dan 326 EK
University of Wisc. Madison
Dept. of Met. & Min. Engineering
1509 University Ave
Madison, WI 53706

Thompson, A.W. 341 WK
Carnegie Mellon University
Dept. of Mems
Pittsburgh, PA 15213

Umakoshi, Yukichi 221 EK
Osaka University
Dept. of Materials Sci. & Eng.
Fac. Eng., 2-1 Yamada-Oka
Suita, Osaka JAPAN 565

Vedulla, Kirshna 324 EK
Case Western Reserve Univ.
6900 Euclid Ave
Metallurgy & Materials Sci.
Cleveland, OH 44106

Veyssiere, Patrick 202 EK
Lab. Metallurgie Physique
Fac. Sciences
40 Avenue, Pineau
Poitiers, FRANCE 86022

Vitek, V. 133 WK
University of Pennsylvania
Dept. of Materials Science & Eng.
Philadelphia, PA 19104

VVedensktly, D.D. 317 EK
Imperial College
Dept. of Physics
London, ENGLAND SW7 2AZ

Ward, Charles 301 EK
Wright-Pqtterson AFB
AFWAL/MLLS
Dayton, Ohio 45433

Weiss, Isaac 134 WK
Wright State University
Dayton, Ohio 45415

Westbrook, J. J. 7 P
Sci-Tech Knowledge Systems
133 Saratoga Road
Scotia, NY 12302

Whang, Sund H. 13 Beau
Polytechnic University
333 Jay Street
Brooklyn, NY 11201

White, Calvin 319 EK
Michigan State University
Dept. of Metal Eng.
Houghton, MI 49931

Williams, James C. 302 EK
CIT, Dean's Office
Carnegie Mellon University
Pittsbrugh, PA 15213

Yamaguchi, Masaharu 1 P
Kyoto University
Dept. of Metal Sciences & Technology
Sakyo-Ku
Kyoto, JAPAN 606

Yaney, Deborah 339 WK
Lockheed California Co.
D/70-13 B/USO P/2
P.O. Box 551
Burbank, CA 91520

Yoo, Man H. 14 Beau
Oak Ridge National Lab.
Oak Ridge, TN 37831

Zordan, Richard 322 EK
Allison Gas Turbine Div. - GM
P.O. Box 420
M/S W-05
Indianapolis, IN 46206-0420

Anton, Donald 227 WK
United Technologies Res. Ctr.
MS 22, Silver Lane
E. Hartford, CT 06108

GORDON RESEARCH CONFERENCES

PHYSICAL METALLURGY
Registration Addendum
July 23, 1987
Tilton School

Blackburn, Martin — 125 WK
Pratt & Whitney
Mil Stop 114-43
400 Main Street
East Hartford, CT 06108

Carpenter, Joseph — off campus
Oak Ridge National Lab
P.O. Box X, Bldg. 4515, MS 065
Oak Ridge, TN 37831

Frost, Harold — 103 EK
Dartmouth College
Thayer School of Engineering
Hanover, NH 03755

Khantha, M. — 335 WK
University of Pennsylvania
c/o Dr. David Pope
Towne Bldg., 220 S., 33rd St.
Philadelphia, PA 19104-6391

Sanchez, J. M. — 19 Beau.
Columbia University
School of Mines
918 Mudd
New York, NY 90027

Sikka, V.K. — 137 WK
Oak Ridge National Lab
P.O. Box X
Oak Ridge, TN 37831

Tien, John — 12 Beau.
Columbia University
Henry Krumb School of Mines
918 S.W. Mudd
New York, NY 10027

END
DATE
FILMD
3-88
DTIC